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1 
$$a: X = S, Y = O, Z = O, n = 0$$

$$b : X = O, Y = CH_2, Z = O, n = 1$$

$$c: X = O, Y = O, Z = CH_2, n = 1$$

$$d: X = S, Y = CH_2, Z = NH, n = 1$$

Fig. 1A

$$2 a : n = 1, X = S$$

$$b : n = 0, X = S$$

$$c : n = 1, X = NH$$

$$d: n = 1, X = 0$$

Fig. 1B

3. 
$$n = 1$$
,  $a : R = hexyl$ ,  $b : R = benzyl$ 

4. 
$$n = 0$$
,  $a : R = hexyl$ ,  $b : R = benzyl$ 

Fig. 1C

нό

ÒН

6. 
$$X = S$$

5 a : Ar =  $p-NO_2-C_6H_4$ 

**b**:  $Ar = p-NH_2-C_6H_4$ 

Fig. 1D

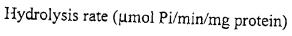
Fig. 1E

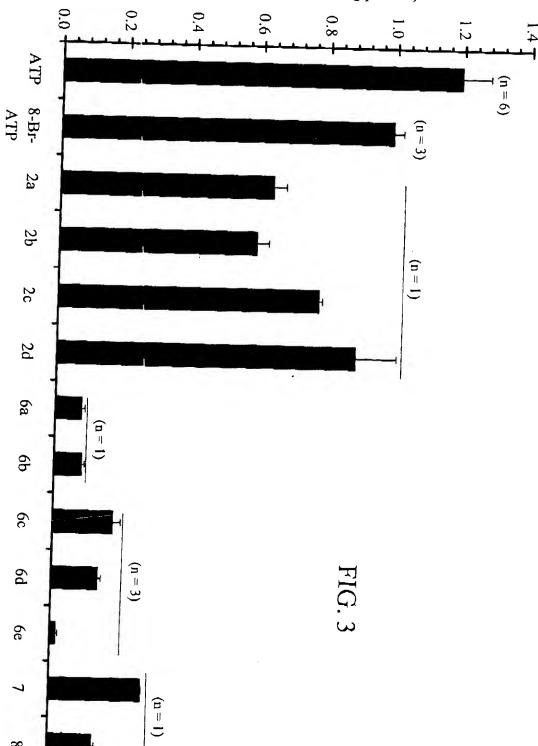
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$$NH_{2}$$
 $NH_{2}$ 
 $N$ 

Fig. 2

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| <u> </u>                      | 4/8                 |                 |                 |                 |                 |                      |                 |                 |                 |                 |
|-------------------------------|---------------------|-----------------|-----------------|-----------------|-----------------|----------------------|-----------------|-----------------|-----------------|-----------------|
| Ki<br>(µM)                    | 31 ± 2.5            | 45 ± 2.5        | $16 \pm 2.0$    | $10 \pm 2.0$    |                 |                      |                 |                 |                 |                 |
|                               | 6a                  | 99              | p9              | 99              |                 |                      |                 |                 |                 |                 |
| Inhibitors                    | 8-cyclohepthylS-ATP | 8-CH2(BuS-ATP   | 8-hexylS-ATP    | 8-BuS-ATP       |                 |                      |                 |                 |                 |                 |
| Vmax<br>(µmol/min/mg protein) | 1.65 ± 0.10         | $1.30 \pm 0.08$ | $0.83 \pm 0.05$ | $0.94 \pm 0.10$ | $0.99 \pm 0.10$ | $0.82 \pm 0.09$      | $0.63 \pm 0.04$ | $0.30 \pm 0.03$ | $0.28 \pm 0.03$ | $0.20 \pm 0.01$ |
| Кт<br>(µМ)                    | 18 ± 1              | 33 ± 1          | 36 ± 6          | 63 ± 14         | 32 ± 8          | <b>28</b> ± <b>8</b> | 22 ± 5          | 12 ± 5          | 20 ± 7          | 26 ± 5          |
|                               |                     |                 | 2a              | 2 <b>b</b>      | 2c              | 24                   |                 | 99              | 7               | 8               |
| Substrates                    | АТР                 | ADP             | 2-BuS-ATP       | 2-BuS-ADP       | 2-BuNH-ATP      | 2-BuO-ATP2d          | 8-bromo-ATP     | 8-cthylS-ATP    | 8-BuNH-ATP      | 8-BuO-ATP       |

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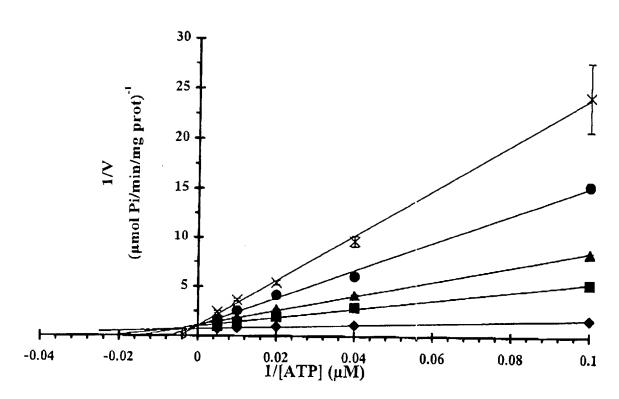
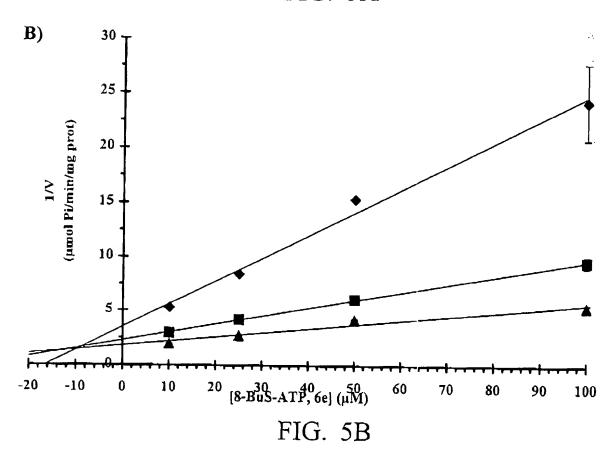


FIG. 5A



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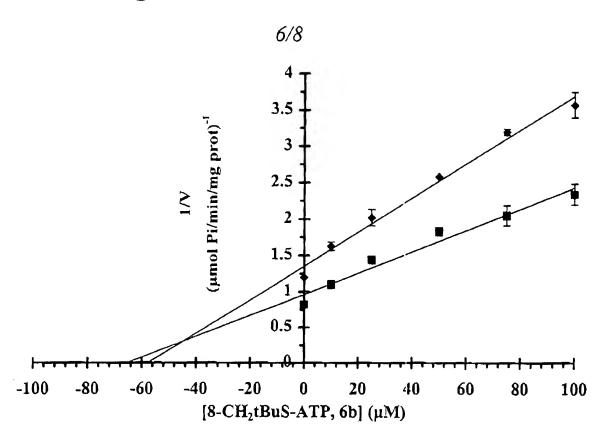
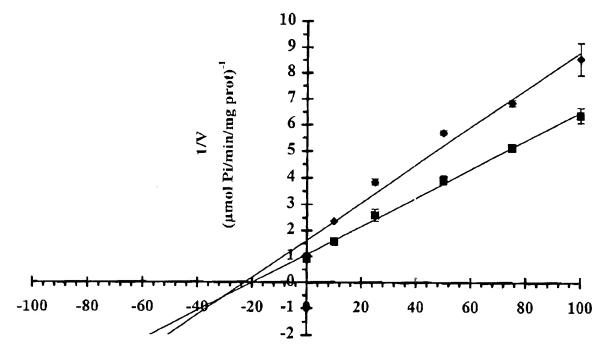


FIG. 6A



[8-cyclohepthylS-ATP, 6a] (µM)

FIG. 6B

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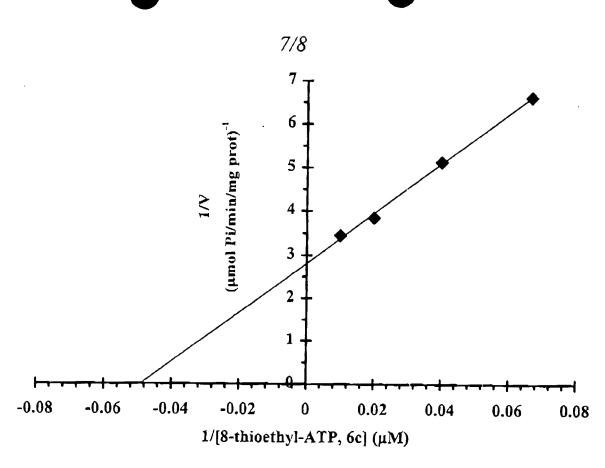


FIG. 7A

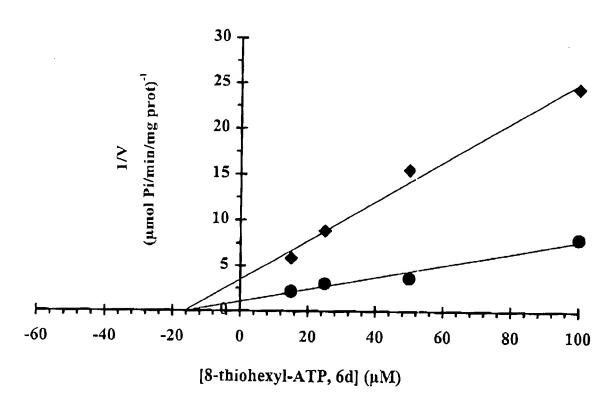


FIG. 7B

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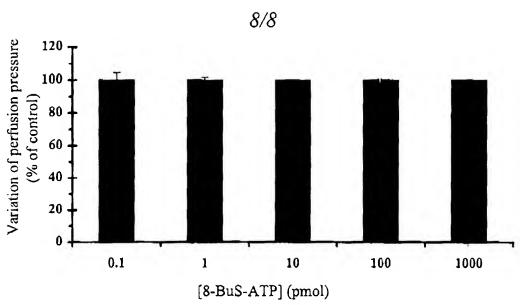
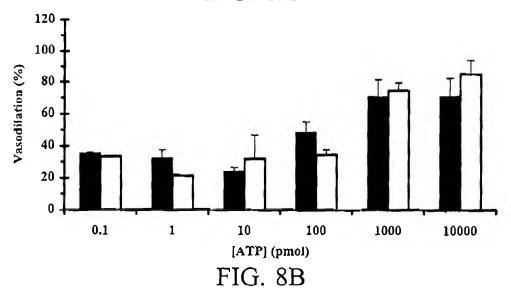


FIG. 8A



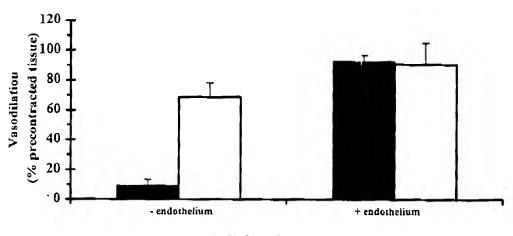


FIG. 8C

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